Inhibition of Hotspot Formation in Polymer Bonded Explosives Using an Interface Matching Low Density Polymer Coating at the Polymer-explosive Interface

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Support Information

Table S1. Bond order cut-off values for various atom pairs. *BondFrag* program uses these values to determine molecular fragments.

	C	**H**	**O**	**N**
C	0.55	0.40	0.80	0.30
H		0.55	0.40	0.55
O			0.65	0.55
N				0.45

ReaxFF Parameters for energetic materials

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39       ! Number of general parameters
  50.0000 !Overcoordination parameter
   9.4514 !Overcoordination parameter
  29.8953 !Valency angle conjugation parameter
 216.5421 !Triple bond stabilisation parameter
  12.2245 !Triple bond stabilisation parameter
   0.0000 !C2-correction
   1.0701 !Undercoordination parameter
   7.5000 !Triple bond stabilisation parameter
  11.9083 !Undercoordination parameter
  13.3822 !Undercoordination parameter
 -10.9834 !Triple bond stabilization energy
   0.0000 !Lower Taper-radius
  10.0000 !Upper Taper-radius
   2.8793 !Not used
  33.8667 !Valency undercoordination
   3.3976 !Valency angle/lone pair parameter
   1.0563 !Valency angle
   2.0384 !Valency angle parameter
   6.1431 !Not used
   6.9290 !Double bond/angle parameter
   0.0283 !Double bond/angle parameter: overcoord
   0.0570 !Double bond/angle parameter: overcoord
  -2.4837 !Not used
   5.8374 !Torsion/BO parameter
  10.0000 !Torsion overcoordination
   1.8820 !Torsion overcoordination
  -1.2327 !Conjugation 0 (not used)
   2.1861 !Conjugation
   1.5591 !vdWaals shielding
   0.0100 !Cutoff for bond order (*100)
   4.8414 !Valency angle conjugation parameter
   3.5857 !Overcoordination parameter
  38.6472 !Overcoordination parameter
   2.1533 !Valency/lone pair parameter
   0.5000 !Not used
  20.0000 !Not used
   5.0000 !Molecular energy (not used)
   0.0000 !Molecular energy (not used)
   6.9784 !Valency angle conjugation parameter
 4    ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
        alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
        cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
        ov/un;val1;n.u.;val3,vval4
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```
C    1.3742   4.0000  12.0000   1.9684   0.1723   0.8712   1.2385   4.0000
     8.7696 100.0000   4.0000  31.0823  79.5548   5.7254   6.9235   0.0000
     1.2104   0.0000 183.8108   5.7419  33.3951  11.9957   0.8563   0.0000
    -2.8983   4.7820   1.0564   4.0000   2.9663   1.6737   0.1421  14.0707
H    0.6867   1.0000   1.0080   1.3525   0.0616   0.8910  -0.1000   1.0000
     9.1506 100.0000   1.0000   0.0000 121.1250   3.8446  10.0839   1.0000
    -0.1000   0.0000  58.4369   3.8461   3.2540   1.0000   1.0698   0.0000
   -15.7683   2.1504   1.0338   1.0000   2.8793   1.2669   0.0139  12.4538
O    1.3142   2.0000  15.9990   1.9741   0.0880   0.8712   1.1139   6.0000
     9.9926 100.0000   4.0000  29.5271 116.0768   8.5000   7.1412   2.0000
     0.9909  14.7235  69.2921   9.1371   1.6258   0.1863   0.9745   0.0000
    -3.5965   2.5000   1.0493   4.0000   2.9225   1.7221   0.1670  13.9991
N    1.2456   3.0000  14.0000   2.0437   0.1035   0.8712   1.1911   5.0000
     9.8823 100.0000   4.0000  32.4758 100.0000   6.8453   6.8349   2.0000
     1.0636   0.0276 127.9672   2.2169   2.8632   2.4419   0.9745   0.0000
    -4.0959   2.0047   1.0183   4.0000   2.8793   1.5967   0.1649  13.9888
10      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                    pbe2;pbo3;pbo4;Etrip;pbo1;pbo2;ovcorr
 1  1 141.9346 113.4487  67.6027   0.1554  -0.3045   1.0000  30.4515   0.4283
       0.0801  -0.2113   8.5395   1.0000  -0.0933   6.6967   1.0000   0.0000
 1  2 163.6889   0.0000   0.0000  -0.4525   0.0000   1.0000   6.0000   0.5921
      12.1053   1.0000   0.0000   1.0000  -0.0097   8.6351   0.0000   0.0000
 2  2 169.8421   0.0000   0.0000  -0.3591   0.0000   1.0000   6.0000   0.7503
       9.3119   1.0000   0.0000   1.0000  -0.0169   5.9406   0.0000   0.0000
 1  3 159.7219 116.8921  77.9315  -0.4324  -0.1742   1.0000  15.0019   0.5160
       1.2934  -0.3079   7.0252   1.0000  -0.1543   4.5116   0.0000   0.0000
 3  3 108.9631 158.3501  42.0558   0.1226  -0.1324   1.0000  28.5716   0.2545
       1.0000  -0.2656   8.6489   1.0000  -0.1000   6.8482   1.0000   0.0000
 1  4 128.9104 171.2945 100.5836  -0.1306  -0.4948   1.0000  26.7458   0.4489
       0.3746  -0.3549   7.0000   1.0000  -0.1248   4.9232   1.0000   0.0000
 3  4  85.0402 118.8680  75.7263   0.7080  -0.1062   1.0000  16.6913   0.2407
       0.3535  -0.1906   8.4054   1.0000  -0.1154   5.6575   1.0000   0.0000
 4  4 160.6599  73.3721 154.2849  -0.7107  -0.1462   1.0000  12.0000   0.6826
       0.9330  -0.1434  10.6712   1.0000  -0.0890   4.6486   1.0000   0.0000
 2  3 219.7016   0.0000   0.0000  -0.6643   0.0000   1.0000   6.0000   0.9854
       5.1146   1.0000   0.0000   1.0000  -0.0532   5.1189   0.0000   0.0000
 2  4 208.0443   0.0000   0.0000  -0.3923   0.0000   1.0000   6.0000   0.3221
      10.5505   1.0000   0.0000   1.0000  -0.0690   6.2949   0.0000   0.0000
6     ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
 1  2   0.0464   1.8296   9.9214   1.0029  -1.0000  -1.0000
 2  3   0.0403   1.6913  10.4801   0.8774  -1.0000  -1.0000
 2  4   0.0524   1.7325  10.1306   0.9982  -1.0000  -1.0000
 1  3   0.1028   1.9277   9.1521   1.3399   1.1104   1.1609
 1  4   0.2070   1.7366   9.5916   1.2960   1.2008   1.1262
 3  4   0.0491   1.7025  10.6101   1.3036   1.1276   1.0173
51    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
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1	1	1	74.0317	32.2712	0.9501	0.0000	0.1780	10.5736	1.0400
1	1	2	70.6558	14.3658	5.3224	0.0000	0.0058	0.0000	1.0400
2	1	2	76.7339	14.4217	3.3631	0.0000	0.0127	0.0000	1.0400
1	2	2	0.0000	0.0000	6.0000	0.0000	0.0000	0.0000	1.0400
1	2	1	0.0000	3.4110	7.7350	0.0000	0.0000	0.0000	1.0400
2	2	2	0.0000	27.9213	5.8635	0.0000	0.0000	0.0000	1.0400
1	1	3	65.1700	8.0170	7.5000	0.0000	0.2028	10.0000	1.0400
3	1	3	71.7582	26.7070	6.0466	0.0000	0.2000	0.0000	1.8525
1	1	4	65.4228	43.9870	1.5602	0.0000	0.2000	10.0000	1.8525
3	1	4	73.7046	23.8131	3.9811	0.0000	0.2000	0.0000	1.8525
4	1	4	65.6602	40.5852	1.8122	0.0000	0.2000	0.0000	1.8525
2	1	3	56.4426	17.6020	5.3044	0.0000	0.9699	0.0000	1.1272
2	1	4	71.0777	9.1462	3.4142	0.0000	0.9110	0.0000	1.0400
1	2	4	0.0000	0.0019	6.3000	0.0000	0.0000	0.0000	1.0400
1	3	1	72.1018	38.4720	1.3926	0.0000	0.4785	0.0000	1.2984
1	3	3	89.9987	44.9806	0.5818	0.0000	0.7472	0.0000	1.2639
1	3	4	70.3281	12.9371	7.5000	0.0000	0.7472	0.0000	1.2639
3	3	3	84.2807	24.1938	2.1695	-10.0000	0.7472	0.0000	1.2639
3	3	4	84.2585	44.1039	0.9185	0.0000	0.7472	0.0000	1.2639
4	3	4	74.2312	25.7005	4.3943	0.0000	0.7472	0.0000	1.2639
1	3	2	89.0416	36.9460	0.4569	0.0000	2.7636	0.0000	2.0494
2	3	3	81.1709	4.2886	6.5904	0.0000	3.0000	0.0000	1.2618
2	3	4	75.9203	44.9675	0.8889	0.0000	3.0000	0.0000	1.2618
2	3	2	82.2020	12.7165	3.9296	0.0000	0.2765	0.0000	1.0470
1	4	1	68.3788	18.3716	1.8893	0.0000	2.4132	0.0000	1.3993
1	4	3	86.5585	37.6814	1.1611	0.0000	1.7325	0.0000	1.0440
1	4	4	74.4818	12.0954	7.5000	0.0000	1.7325	0.0000	1.0440
3	4	3	78.5850	44.3389	1.3239	-26.2246	1.7325	40.0000	1.0440
3	4	4	77.6245	32.0866	1.8889	-0.9193	1.7325	0.0000	1.0440
4	4	4	66.4718	15.9087	7.5000	0.0000	1.7325	0.0000	1.0440
1	4	2	90.0000	33.6636	1.1051	0.0000	0.2638	0.0000	1.1376
2	4	3	83.8493	44.9000	1.3580	0.0000	0.5355	0.0000	2.5279
2	4	4	78.7452	24.2010	3.7481	0.0000	0.5355	0.0000	2.5279
2	4	2	55.8679	14.2331	2.9225	0.0000	0.2000	0.0000	2.9932
1	2	3	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
1	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
1	2	5	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
3	2	3	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
3	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
4	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
2	2	3	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
2	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
1	1	5	74.4180	33.4273	1.7018	0.1463	0.5000	0.0000	1.6178
1	5	1	79.7037	28.2036	1.7073	0.1463	0.5000	0.0000	1.6453
2	1	5	63.3289	29.4225	2.1326	0.0000	0.5000	0.0000	3.0000
2	3	6	83.7634	5.6693	2.7780	0.0000	1.6982	0.0000	1.0400

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 3  3  6  73.4663  25.0761   0.9143   0.0000   2.2466   0.0000   1.0400
 2  2  6   0.0000  47.1300   6.0000   0.0000   1.6371   0.0000   1.0400
 6  2  6   0.0000  31.5209   6.0000   0.0000   1.6371   0.0000   1.0400
 3  2  6   0.0000  31.0427   4.5625   0.0000   1.6371   0.0000   1.0400
 2  2  5   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
25    ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
 1  1  1  1   0.0000  48.4194   0.3163  -8.6506  -1.7255   0.0000   0.0000
 1  1  1  2   0.0000  63.3484   0.2210  -8.8401  -1.8081   0.0000   0.0000
 2  1  1  2   0.0000  45.2741   0.4171  -6.9800  -1.2359   0.0000   0.0000
 0  1  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  2  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  1  3  0   1.7254  86.0769   0.3440  -4.2330  -2.0000   0.0000   0.0000
 0  2  3  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000   0.0000
 0  3  3  0   1.2314 116.5137   0.5599  -4.1412   0.0000   0.0000   0.0000
 0  1  4  0  -1.3258 149.8644   0.4790  -7.1541  -2.0000   0.0000   0.0000
 0  2  4  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000   0.0000
 0  3  4  0   1.3168  57.0732   0.2679  -4.1516  -2.0000   0.0000   0.0000
 0  4  4  0   2.0000  75.3685  -0.7852  -9.0000  -2.0000   0.0000   0.0000
 0  1  1  0   0.0930  18.6070  -1.3191  -9.0000  -1.0000   0.0000   0.0000
 4  1  4  4  -2.0000  20.6655  -1.5000  -9.0000  -2.0000   0.0000   0.0000
 1  1  3  3   1.2707  21.6200   1.5000  -9.0000  -2.0000   0.0000   0.0000
 1  3  3  1  -1.8804  79.9255  -1.5000  -4.1940  -2.0000   0.0000   0.0000
 3  1  3  3  -2.0000  22.5092   1.5000  -8.9500  -2.0000   0.0000   0.0000
 1  4  4  3   0.1040  70.1152   0.5284  -3.5026  -2.0000   0.0000   0.0000
 1  1  3  4   1.2181 119.6186  -1.5000  -7.0635  -2.0000   0.0000   0.0000
 2  1  3  4  -2.0000 156.6604   1.1004  -7.3729  -2.0000   0.0000   0.0000
 1  3  4  3   2.0000  96.6281  -1.5000  -3.8076  -2.0000   0.0000   0.0000
 1  1  4  2  -2.0000 147.2445  -1.5000  -7.0142  -2.0000   0.0000   0.0000
 1  1  4  3  -2.0000  47.8326  -1.5000  -9.0000  -2.0000   0.0000   0.0000
 2  3  4  3  -0.2997 152.9040  -1.5000  -4.4564  -2.0000   0.0000   0.0000
 2  4  4  3   0.1040  70.1152   0.5284  -3.5026  -2.0000   0.0000   0.0000
 4    ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
 3  2  3   2.1845  -2.3549   3.0582  19.1627
 3  2  4   1.6658  -3.8907   3.0582  19.1627
 4  2  3   1.8738  -3.5421   3.0582  19.1627
 4  2  4   1.8075  -4.1846   3.0582  19.1627
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